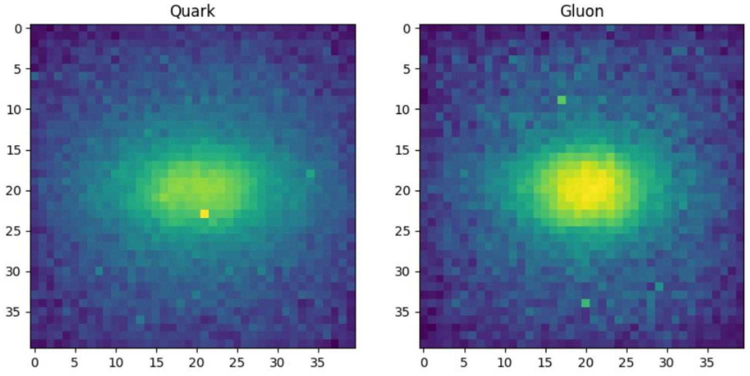
Google Summer of Code

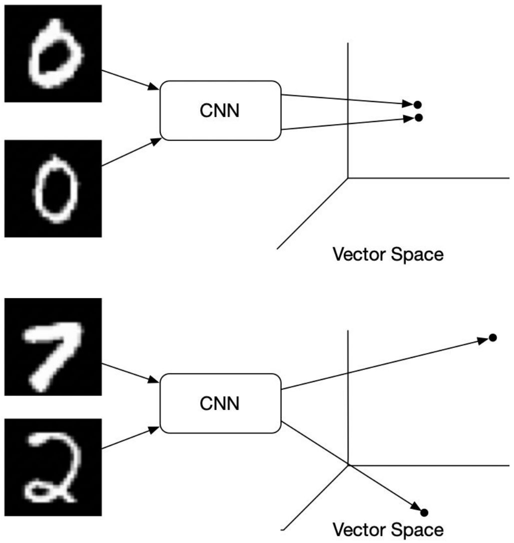
Sanya Nanda

Machine Learning for Science (ML4Sci)

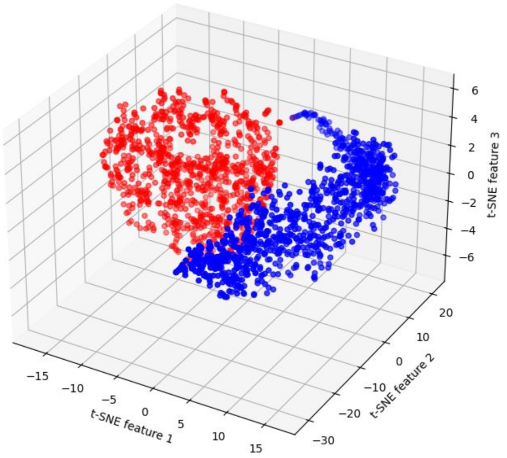
Project Objective: Learning quantum representations of classical high energy physics data with contrastive learning



High Energy Physics Data:
Quark-Gluon (Avg of Tracks channel)



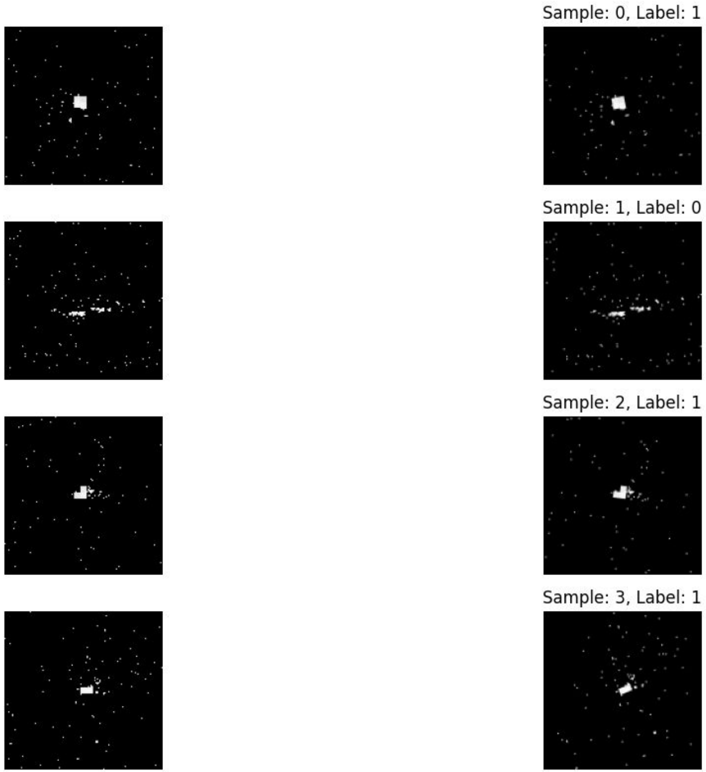
Contrastive Learning



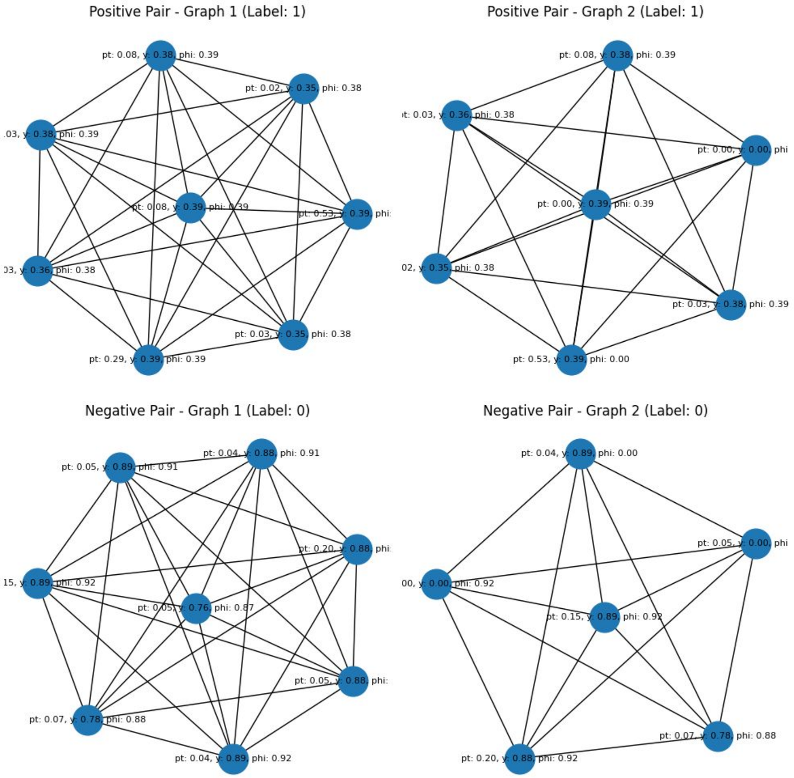
Representation embeddings

python TensorFlow PyTorch PENNYLANE W&B

Positive Negative Views

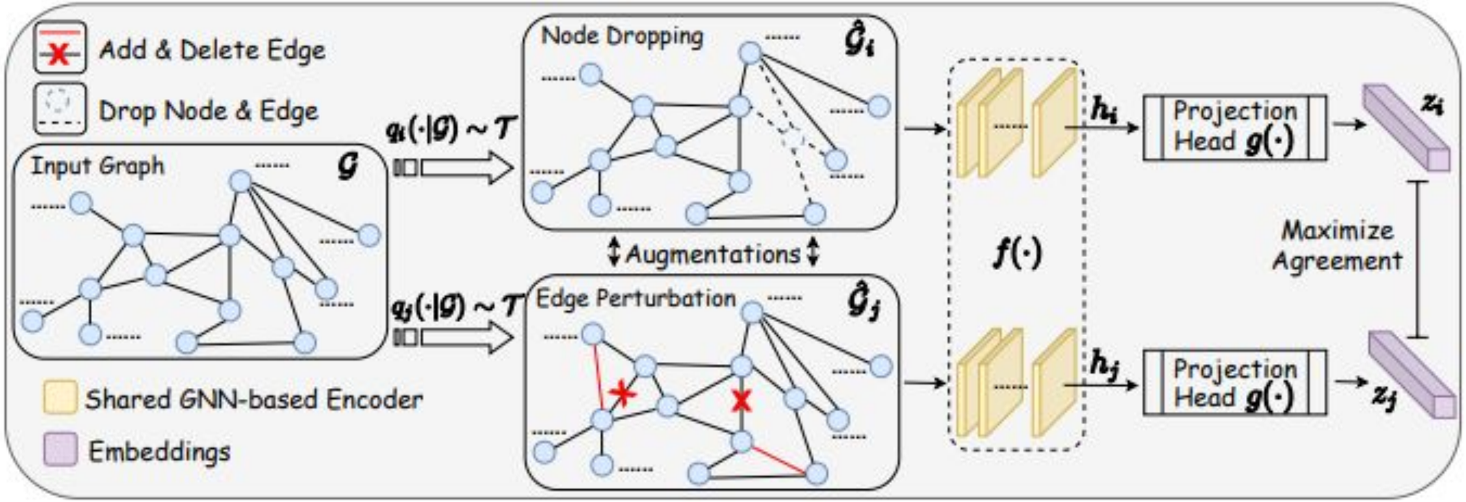


Quark-Gluon: image pairs



Quark-Gluon: graph pairs

Model Architecture & Loss Functions



Ref: You, Y., Chen, T., Sui, Y., Chen, T., Wang, Z. and Shen, Y., 2020. Graph contrastive learning with augmentations. Advances in neural information processing systems, 33, pp.5812-5823.

$$\mathcal{L} = y \cdot D^2 + (1-y) \cdot \max(0, m - D)^2$$

Contrastive Pair Loss

$$\mathcal{L}_{\text{InfoNCE}} = -\log \frac{\exp(\text{sim}(z_i, z_j)/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{k \neq i} \exp(\text{sim}(z_i, z_k)/\tau)}$$

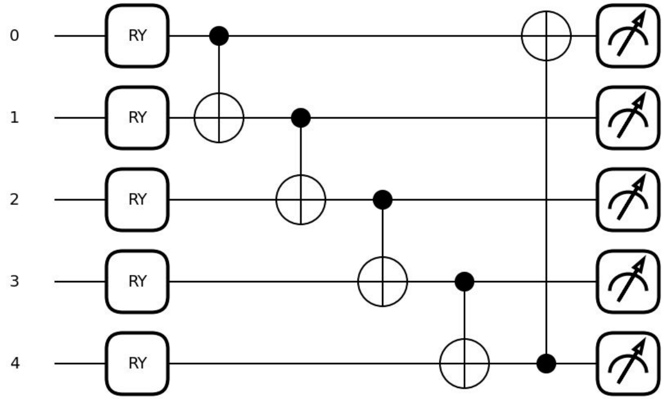
InfoNCE Loss

$F(\rho_1, \rho_2) = |\langle \psi_1 | \psi_2 \rangle|^2$ where $|\psi_1\rangle$ and $|\psi_2\rangle$

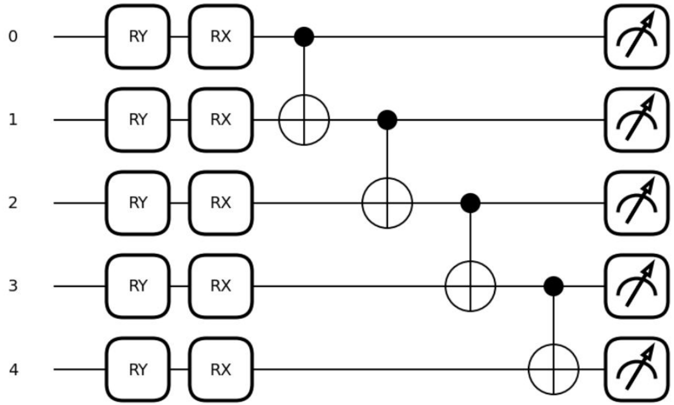
$$\mathcal{L}\text{total} = \alpha \mathcal{L}\text{InfoNCE} + (1-\alpha)(1 - F(\rho_1, \rho_2))$$

InfoNCE Loss + Fidelity

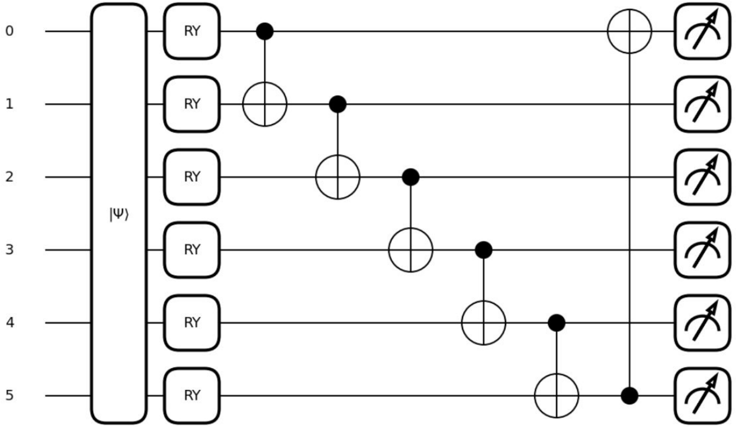
Quantum circuits as Projection Heads



Ry Rotations + Entanglement

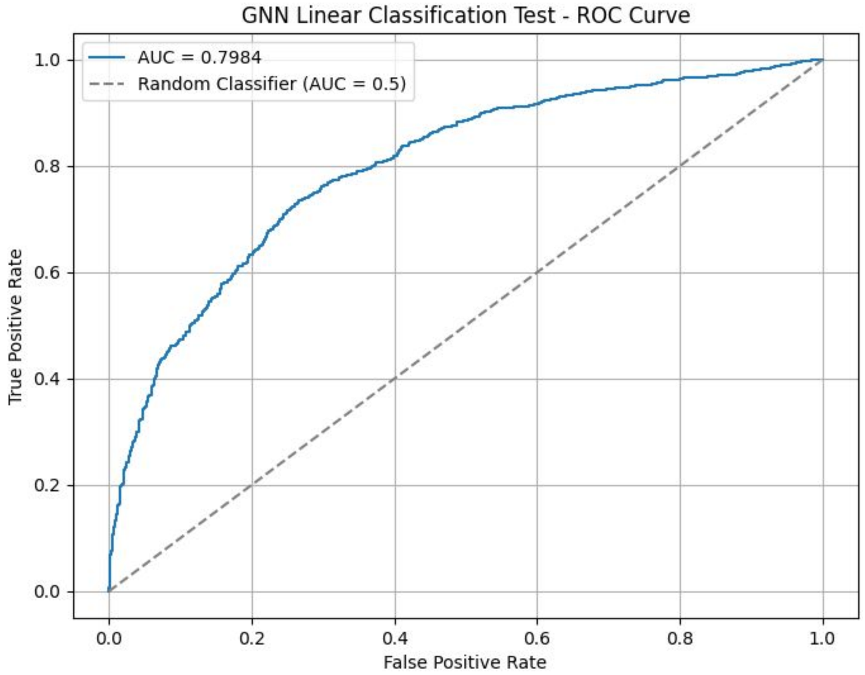


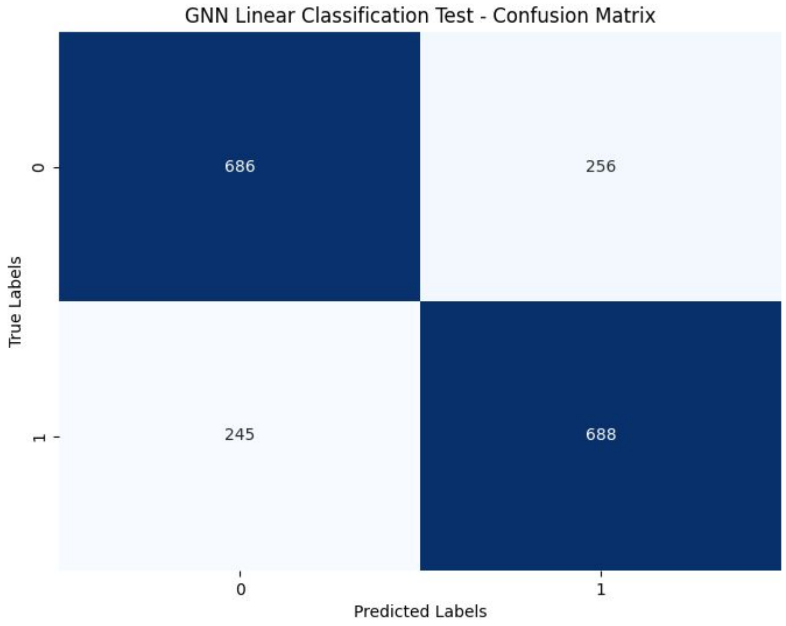
Angle Embedding + Entanglement



Amplitude Embedding + Entanglement

Model Evaluation





Benchmarking

Dataset	Model	Validation Loss	Validation Accuracy
0-1 MNIST	CNN Encoder + contrastive pair	0.000911	0.9997
3-8 MNIST	CNN Encoder + contrastive pair	0.004080	0.9977
9-6 MNIST	CNN Encoder + contrastive pair	0.002580	0.9994
Quark-Gluon	CNN Encoder + contrastive pair	0.4921	0.5617

Table 1: CNN encoder on MNIST and Quark-Gluon

Model	Test Accuracy (%)	AUC
CNN Encoder	56.17%	0.52
ResNet18 Encoder	60.02%	0.5416
GNN Encoder	73.28%	0.7984

Table 2: Different classical encoders on Quark-Gluon

Model	Test Accuracy (%)	AUC
GNN Encoder	73.28%	0.7984
GNN Encoder + Quantum projection head (QC1)	66.93%	0.7287
GNN Encoder + (QC2) + Fidelity	60.37%	0.6448
GNN Encoder + QC3	67.02%	0.7285

Table 3: Classical and Quantum GNN on Quark-Gluon

Conclusion

Future Scope

Experimenting with fully quantum model and applying contrastive learning to more HEP datasets

Learnings

Technical Growth: I dived deep into coding machine learning workflows, while refining my skills in writing clean, efficient code.

Personal Development: Through our weekly sync-up calls, I immensely improved my presentation skills and also connected with a wonderful global community.

"The best part of GSoC; the people I met - mentors, peers and contributors who shaped this journey with shared experiences, learnings and camaraderie "

Thank You!